

Adiabatic Approximation Condition

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In this paper, we present an invariant perturbation theory of the adiabatic process based on the concepts of $U(1)$ -invariant adiabatic orbit and $U(1)$ -invariant adiabatic expansion. As its application, we propose and discuss new adiabatic approximation conditions.

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Since the establishment of the quantum adiabatic theorem [1,2,3,4] in 1923, many fundamental results have been obtained, such as Landau-Zener transition [5], the Gell-Mann-Low theorem [6], Berry phase [7] and holonomy [8]. Also the adiabatic processes find their applications in the quantum control and quantum computation [9,10,11,12]. Recently the common-used quantitative adiabatic condition [15,16,17] has been found not able to guarantee the validity of the adiabatic approximation [13,14]. Consequently various new conditions are conjectured and a series of confusions and debates arise. For example, it was argued [18] that the traditional adiabatic condition did not have any problem at all and that the invalidation of the condition did not mean the invalidation of adiabatic theorem [19]. Some new conditions proposed in [20,21] but too rigorous to be used conveniently. Although [22] also adopted the adiabatic perturbation expansion but did not give out proper condition because the basis in [22] can not show certain geometric properties in the adiabatic process. [23] pointed out the limitation of traditional condition but also did not give out a proper condition. To solve the problem of insufficiency of traditional adiabatic condition in [13,14] and clarify the subsequent confusions, we introduce the concepts of *adiabatic orbit*, *$U(1)$ -invariant adiabatic orbit* and *$U(1)$ -invariant adiabatic evolution orbit*. The meanings of adiabatic evolution is reclaimed. And new adiabatic approximation conditions based on the *$U(1)$ -invariant adiabatic expansion* with the time-dependent coefficient are proposed and illustrated by two examples.

Let us consider a quantum system governed by a time dependent Hamiltonian $H(t)$ and the initial state of the system is an eigenstate $|m, 0\rangle$ of $H(0)$ with eigenvalue $E_m(0)$, where m denotes the initial value of dimensionless quantum number set. By introducing a dimensionless time parameter $\tau = E_m(0)t/\hbar$ and a dimensionless Hamiltonian $h(\tau) = H(\tau)/E_m(0)$, the time dependent Schrödinger equation reads

$$i \frac{\partial |\Phi_m(\tau)\rangle}{\partial \tau} = h(\tau) |\Phi_m(\tau)\rangle, \quad |\Phi_m(0)\rangle = |m, 0\rangle. \quad (1)$$

The exact solution $|\Phi_m(\tau)\rangle$ to Eq.(1) is referred to as the system's *dynamic evolution orbit* in the Hilbert space.

Furthermore, by considering τ as a fixed parameter, we can always solve the following quasi-stationary equation of the

Hamiltonian $h(\tau)$

$$h(\tau) |\varphi_n(\tau)\rangle = e_n(\tau) |\varphi_n(\tau)\rangle. \quad (2)$$

And the eigenstate $|\varphi_n(\tau)\rangle$ with the corresponding initial state $|n, 0\rangle$ is referred to as the *adiabatic solution* or the *adiabatic orbit* of the system.

For convenience, we denote $\gamma_{nm} \equiv i \langle \varphi_n(\tau) | \dot{\varphi}_m(\tau) \rangle$ and the dot here and below expresses the derivative with respect to time. Apparently, an adiabatic orbit multiplied by an arbitrary time-dependent phase factor still describes the same adiabatic orbit. It is not difficult to see that the following adiabatic orbit

$$|\Phi_m^{adia}(\tau)\rangle = \exp \left\{ -i \int_0^\tau [e_m(\lambda) - \gamma_{mm}(\lambda)] d\lambda \right\} |\varphi_m(\tau)\rangle \quad (3)$$

is invariant [26] under the following $U(1)$ transformation

$$|\varphi_m(\tau)\rangle \rightarrow e^{if_m(\tau)} |\varphi_m(\tau)\rangle \quad (f_m(0) = 0). \quad (4)$$

Here $f_m(0) = 0$ is because of given initial state. We call this adiabatic orbit with special choice of the time-dependent phase factor as the *$U(1)$ -invariant adiabatic orbit*.

It is clear that, although the initial conditions $|m, 0\rangle$ are the same, the dynamic evolution orbit $|\Phi_m(\tau)\rangle$ do not always coincide with the adiabatic orbit $|\varphi_m(\tau)\rangle$, or they are not even close to each other. Obviously they coincide if and only if

$$\gamma_{nm} = 0 \quad (\forall n \neq m). \quad (5)$$

In this case, Eq.(3) being the solution to both Eq.(1) and Eq.(2) is referred to as the *$U(1)$ -invariant adiabatic evolution orbit*, describing a strict adiabatic evolution orbit of the system.

Generally speaking, the dynamic evolution orbit $|\Phi_m(\tau)\rangle$ starting from the initial state $|m, 0\rangle$ will change among some adiabatic orbits which will cause transitions between different them. Our task is to find the proper condition under which the dynamic orbit is sufficiently close to the adiabatic orbit when the Eq.(5) is not satisfied.

Since the Hamiltonian $h(\tau)$ is Hermitian, all the *$U(1)$ -invariant adiabatic orbits* in Eq.(3) at a given time constitute a complete orthonormal basis of the system. In this basis, the dynamic evolution orbit of system reads

$$|\Phi_m(\tau)\rangle = \sum_n c_n(\tau) |\Phi_n^{adia}(\tau)\rangle, \quad |\Phi_m(0)\rangle = |m, 0\rangle. \quad (6)$$

The expansion in Eq.(6) is referred to as the $U(1)$ -invariant adiabatic expansion with the time-dependent coefficients. Therefore, the set of coefficients equations reads

$$\dot{c}_m(\tau) = i \sum_{n \neq m} c_n(\tau) M(\tau)_{mn}, \quad (7)$$

where the diagonal elements of the matrix $M(\tau)$ are zero and the non-diagonal elements of $M(\tau)$ read

$$M(\tau)_{mn} = i \langle \Phi_m^{adi}(\tau) | \dot{\Phi}_n^{adi}(\tau) \rangle \equiv |\gamma_{nm}(\tau)| e^{i\theta_{nm}(\tau)}, \quad (8)$$

where

$$\theta_{nm}(\tau) = \int_0^\tau d\lambda (e_m(\lambda) - e_n(\lambda) + \gamma_{nn} - \gamma_{mm}) + \arg \gamma_{nm}(\tau). \quad (9)$$

Thus, the probability of staying in adiabatic orbit $|\Phi_m^{adia}(\tau)\rangle$ is

$$P_m(\tau) = |c_m(\tau)|^2 = \left| \left(\hat{T} \exp \left[i \int_0^\tau d\lambda M(\lambda) \right] \right)_{mm} \right|^2, \quad (10)$$

where \hat{T} is time ordered operator. And one can obtain further detailed analysis on Eq.(10) in our another paper [24].

Accordingly, the adiabatic approximation of system requires

$$P_m(\tau) \rightarrow 1. \quad (11)$$

It means the transition probability from dynamic evolution orbit to other adiabatic orbits (except the adiabatic orbit $|\Phi_m^{adia}(\tau)\rangle$) can be neglected.

According to the perturbation theory for Eq.(10), the first-order approximation of $P_m(\tau)$ is

$$P_m(\tau) = 1 - \sum_{n \neq m} \left| \int_0^\tau |\gamma_{nm}(\lambda)| e^{i\theta_{nm}(\lambda)} d\lambda \right|^2. \quad (12)$$

Therefore, the adiabatic approximation requires

$$\left| \int_0^\tau |\gamma_{nm}(\lambda)| e^{i\theta_{nm}(\lambda)} d\lambda \right|^2 \rightarrow 0 \quad (\forall n \neq m). \quad (13)$$

For general situation $|\theta_{nm}(\tau) - \theta_{nm}(0)| \geq 2\pi$ and $|\dot{\theta}_{nm}(\tau)| \geq 1$, the integral of Eq.(13) will be sufficiently small, if the phase of the integrated function vibrates fast enough and the amplitude of the integrated function is small enough, thus we will have following adiabatic condition

$$|\dot{\theta}_{nm}(\tau)| \gg |\gamma_{nm}(\tau)| \quad (\forall n \neq m) \quad (14)$$

that is

$$|e_n(\tau) - e_m(\tau) + \Delta_{mn}(\tau)| \gg |\gamma_{nm}(\tau)| \quad (\forall n \neq m) \quad (15)$$

where

$$\Delta_{mn}(\tau) \equiv \gamma_{mm}(\tau) - \gamma_{nn}(\tau) + \frac{d}{d\tau} \arg \gamma_{nm}(\tau) \quad (\forall n \neq m). \quad (16)$$

Here Δ_{mn} referred to as *quantum geometric potential* is a new quantity comparing to the traditional adiabatic condition. And it should be noticed [26] that the *quantum geometric potential* is also $U(1)$ -invariant under the transformation Eq.(4). It should point out that Δ_{mn} appears naturally in our theory. And for *quantum geometric potential* one can obtain further detailed analysis and application in our another paper [25]. Furthermore, from Eq.(13), the change of the phase in the integrated function should be much larger than the integral of amplitude, we will have another condition in integral form

$$\left| \int_0^\tau d\lambda [e_n(\lambda) - e_m(\lambda) + \Delta_{mn}] \right| \gg \int_0^\tau d\lambda |\gamma_{nm}(\lambda)|, \quad \forall n \neq m. \quad (17)$$

Based on Eq.(7) and Eq.(8), we also prove [27] a theorem related to condition Eq.(14) and Eq.(17). Following analysis and our subsequent works [24,25] indicate that Eq.(9-18) are of abundant content.

Next we will give two examples to show the validity of Eq.(15) and Eq.(17).

The first example is to indicate that the problems shown in [13,14] do not exist because the relation between system a and b stated in Ref.[13,14] does not guarantee our condition Eq.(15). The proof is given below.

[14] showed that for an arbitrary time-dependent system a with Hamiltonian $h^a(\tau)$ and quasi-stationary equation $h^a(\tau) |n^a(\tau)\rangle = e_n^a(\tau) |n^a(\tau)\rangle$, one can construct time-dependent system b with Hamiltonian $h^b(\tau)$ and quasi-stationary equation $h^b(\tau) |n^b(\tau)\rangle = e_n^b(\tau) |n^b(\tau)\rangle$ as follows

$$\begin{cases} h^a(\tau) = i\dot{U}(\tau)U^\dagger(\tau), h^b(\tau) = i\dot{U}^\dagger(\tau)U(\tau) \\ |n^b(\tau)\rangle = U^\dagger(\tau) |n^a(\tau)\rangle, \quad e_n^b(\tau) = -e_n^a(\tau). \end{cases} \quad (18)$$

Simple calculation yields

$$\gamma_{nm}^b(\tau) = -e_m^a(\tau)\delta_{mn} + \gamma_{nm}^a(\tau). \quad (19)$$

Using Eq.(15), we have

$$\frac{|\gamma_{nm}^a(\tau)|}{|e_m^a(\tau) - e_n^a(\tau) - \Delta_{mn}^a(\tau)|} \ll 1, \quad \forall n \neq m \quad (20)$$

for system a , while for system b , we will have

$$\frac{|\gamma_{nm}^b(\tau)|}{|e_m^b(\tau) - e_n^b(\tau) - \Delta_{mn}^b(\tau)|} = \frac{|\gamma_{nm}^a(\tau)|}{|\Delta_{mn}^a(\tau)|}. \quad (21)$$

Comparing adiabatic conditions between system a Eq.(20) and system b Eq.(21), the denominator of Eq.(20) has an extra term $e_m^a(\tau) - e_n^a(\tau)$. Therefore, we can not conclude that system

b still satisfies Eq.(15). This indicates that the problems stated in [13,14] will not exist if we adopt the new adiabatic condition Eq.(15). And it is worthwhile to point out that we can present accurate adiabatic condition for the examples given in [14] according to our condition Eq.(15).

The second example is to consider the well-known model, a spin-half particle in a general magnetic field. The Hamiltonian of the system is

$$h(\tau) = \eta \sigma_z + \xi(\tau) (\sigma_x \cos 2\eta\tau + \sigma_y \sin 2\eta\tau) \quad (22)$$

where $\eta = \hbar\omega_0/E_{\pm}(0)$, $\xi(\tau) = \hbar\omega(\tau)/E_{\pm}(0)$ and ω_0 is a constant. Suppose that the initial state of the system is $|\pm, 0\rangle = \exp(-i\sigma_y\theta(0)/2)|\pm\vec{e}_z\rangle$ with energy eigenvalues $E_{\pm}(0)$ at initial time respectively, where $\theta(0) = \arctan(\omega(0)/\omega_0)$ and $|\pm\vec{e}_z\rangle$ are the eigenstates of σ_z . The dynamic evolution orbits of the system are

$$|\Phi_{\pm}(\tau)\rangle = e^{-i\sigma_z\eta\tau} e^{-i\sigma_x \int_0^\tau \xi(\lambda)d\lambda} |\pm, 0\rangle. \quad (23)$$

Here, the two $U(1)$ -invariant adiabatic orbits passing through the corresponding initial eigenstates $|\pm, 0\rangle$ are

$$|\Phi_{\pm}^{adia}(\tau)\rangle = e^{-i\eta\tau\sigma_z} e^{-i\theta(\tau)\sigma_y/2} e^{-i\sigma_x \int_0^\tau (\Omega(\lambda) - \frac{\eta^2}{\Omega(\lambda)})d\lambda} |\pm\vec{e}_z\rangle, \quad (24)$$

here $\Omega(\tau) = \sqrt{\xi(\tau)^2 + \eta^2}$, $\cos\theta(\tau) = \eta/\Omega(\tau)$ and $|\Phi_{\pm}^{adia}(0)\rangle = |\pm, 0\rangle$.

Now, we use the new adiabatic condition Eq.(17) to examine under what circumstances the evolution of the system keeps in the adiabatic orbit, $|\Phi_{+}^{adia}(\tau)\rangle$. First of all, it is easy to calculate the probability of finding the dynamic evolution orbit of the system in the adiabatic orbit $|\Phi_{+}^{adia}(\tau)\rangle$

$$P_m = \left| \langle \Phi_{+}^{adia}(\tau) | \Phi_{+}(\tau) \rangle \right|^2 = \frac{1}{2} + \frac{1}{2} \frac{\xi(0)\xi(\tau) + \eta^2 \cos 2\delta}{\Omega(0)\Omega(\tau)}, \quad (25)$$

where $\delta = -\int_0^\tau \xi(\lambda)d\lambda$.

Suppose that $|\theta_{-+}(\tau)| \geq 1$ and $|\theta_{-+}(\tau) - \theta_{-+}(0)| \geq 2\pi$, then according to the condition Eq.(17), we will have

$$\begin{aligned} & \left| 2 \int_0^\tau d\lambda \frac{\xi(\lambda)^2}{\Omega(\lambda)} - \left(\arg \gamma_{-+}(\lambda) \right)_0^\tau \right| \\ & \gg \int_0^\tau d\lambda \frac{\eta\xi(\lambda)}{\Omega(\lambda)} \sqrt{\frac{\xi(\lambda)^2}{4\Omega(\lambda)^2\xi(\lambda)^2} + 1}. \end{aligned} \quad (26)$$

After simple analysis, we will obtain following sufficient condition

$$\xi(\tau) \gg \eta \quad (27)$$

or

$$\eta \gg \xi(\tau) \text{ and } \int_0^\tau \xi(\lambda)d\lambda \ll 1. \quad (28)$$

It is easy to see that when Eq.(27) or Eq.(28) is satisfied, from Eq.(25), we have

$$P_m = \left| \langle \Phi_{+}^{adia}(\tau) | \Phi_{+}(\tau) \rangle \right|^2 \approx 1. \quad (29)$$

Namely, our new adiabatic condition Eq.(17) guarantees the evolution of the system is an adiabatic evolution. What is more, we can choose proper $\xi(\tau)$ to be periodic, so the condition stated in Ref.[20] can not be applied to our example and has obvious limitation. In fact, the adiabatic process may be a longtime vibration process, so the condition influenced by the times of vibration stated in Ref.[20] is too much strict. As for the general sufficient condition stated in Ref.[21], it is not only too complicated to operate but also too rigorous to apply.

In conclusion, according to the concepts of adiabatic orbit, $U(1)$ -invariant adiabatic orbit and adiabatic evolution orbit stated in our paper, we reclaim the meanings of adiabatic evolution and present an invariant perturbation theory of adiabatic process based on time-dependent $U(1)$ invariant adiabatic expansion. Of course, Eq.(15) and Eq.(17) can not be proved to be sufficient condition, thus we give out sufficient conditions in [27] which contains Eq.(15) and Eq.(17), however, the second condition in [27] are too strict to exclude many interesting physical systems. As far as we know, the conditions Eq.(15) and Eq.(17) can be used to determine whether the evolution of the system is adiabatic or not for all familiar examples listed in the existed papers. We also preliminarily show the influence of quantum geometric potential in the new adiabatic condition. Further detailed discussions on quantum geometric potential and the new adiabatic conditions can be seen in [24,25].

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 [25] Meisheng Zhao, Jianda Wu, Jianlan Chen, and Yongde Zhang "Properties of Quantum Geometric Potential in The New Adiabatic Approximation Condition".
 [26] Here we will prove that *adiabatic basis* $\{|\Phi_m^{adia}(\tau)\rangle\}$ and *quantum geometric potential* $\Delta_{mn}(\tau)$ are both invariant under arbitrary time-dependent $U(1)$ transformation.
Proof: Perform an arbitrary time-dependent $U(1)$ transformation on adiabatic orbit $|\varphi_n(\tau)\rangle$

$$|\varphi_n(\tau)\rangle \rightarrow |\varphi'_n(\tau)\rangle = e^{i f_n(\tau)} |\varphi_n(\tau)\rangle. \quad (30)$$

Thus, we will have

$$e^{-i \int_0^\tau [e_m(\lambda) - \gamma_{mn}(\lambda)] d\lambda} |\varphi'_m(\tau)\rangle = e^{i f_m(0)} e^{-i \int_0^\tau [e_m(\lambda) - \gamma_{mn}(\lambda)] d\lambda} |\varphi_m(\tau)\rangle \quad (31)$$

The given phase of initial state $|m, 0\rangle$ requires $f_m(0) = 0$. Thus we prove adiabatic basis $\{|\Phi_m^{adia}(\tau)\rangle\}$ is $U(1)$ -invariant. And the proof for $\Delta_{mn}(\tau)$ is similar. Performing the same $U(1)$ transformation, we will have

$$\begin{aligned} \Delta'_{mn}(\tau) &= [\gamma_{mn}(\tau) - \dot{f}_m(\tau)] - [\gamma_{nn}(\tau) - \dot{f}_n(\tau)] \\ &\quad + \frac{d}{d\tau} \arg \left[i \langle \varphi_n(\tau) | e^{-i f_n(\tau) + i f_m(\tau)} | \varphi_m(\tau) \rangle \right] \\ &= \Delta_{mn}(\tau) \quad (m \neq n) \end{aligned} \quad (32)$$

These two proofs show that even if the phase $\gamma_{kk}(\tau)$ is dependent of time, we still can use them to construct meaningful quantity which has physical meanings and will not change under any time-dependent $U(1)$ transformation. The quantum geometric potential $\Delta_{mn}(\tau)$ and adiabatic basis $\{|\Phi_m^{adia}(\tau)\rangle\}$ are just the cases. And all these quantities should exist in all time-dependent process. We should note that the traditional Berry phase can be included if we perform cyclic integral on the phase in $\{|\Phi_m^{adia}(\tau)\rangle\}$.

[27] **Theorem** For an N -level quantum system and an arbitrary real ε and a time period T , if the following conditions hold

$$\max_{\tau, n \neq m} \left| \frac{\gamma_{nm}(\tau)}{\theta_{nm}(\tau)} \right| \leq \frac{\varepsilon}{3N} \quad (33)$$

$$\max_{n \neq m} \int_0^T d\tau \left| \frac{d}{d\tau} \left(\frac{\gamma_{nm}(\tau)}{\theta_{nm}(\tau)} \right) \right| \leq \frac{\varepsilon}{3N} \quad (34)$$

$$\max_{n \neq m, l \neq n} \int_0^T d\tau |\dot{\theta}_{ln}(\tau)| \leq \frac{3}{\varepsilon} \quad (35)$$

then the probability of finding dynamical orbit in the adiabatic orbit $|\Phi_m^{adi}(\tau)\rangle$ is greater than $(1 - \varepsilon)^2$.

Proof: From Eq.(7) and Eq.(8), we have

$$\begin{aligned} c_m(T) - 1 &= i \sum_{n \neq m} \int_0^T d\tau |\gamma_{mn}(\tau)| e^{-i\theta_{mn}(\tau)} c_n(\tau) \\ &= \sum_{n \neq m} \frac{|\gamma_{mn}|}{\dot{\theta}_{mn}} e^{i\theta_{mn}} c_n(\tau) \Big|_0^T - \sum_{n \neq m} \int_0^T d\tau \frac{d}{d\tau} \left(\frac{|\gamma_{mn}|}{\dot{\theta}_{mn}} \right) e^{i\theta_{mn}} c_n(\tau) \\ &\quad - i \sum_{n \neq m, l \neq n} \int_0^T d\theta_{nl}(\tau) \frac{|\gamma_{mn}|}{\dot{\theta}_{mn}} \frac{|\gamma_{nl}|}{\dot{\theta}_{nl}} e^{i(\theta_{mn} + \theta_{nl}(\tau))} c_l(\tau). \end{aligned} \quad (36)$$

Then from Eq.(33), Eq.(34) and Eq.(35), we have

$$1 - |c_m(\tau)| \leq |1 - c_m(\tau)| \leq \varepsilon \quad (37)$$

namely,

$$P_m = |c_m(\tau)|^2 \geq (1 - \varepsilon)^2. \quad (38)$$

Thus we prove the theorem.